C:\Documents and Settings\KPuttlitz\My Documents\09486981rxn1.str chain nodes : 7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 32 33 36 37 38 39 40 41 ring nodes : 1 2 3 4 5 6 16 17 18 19 20 chain bonds : ring bonds : . 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 exact/norm bonds : 2-12 12-13 13-14 18-27 exact bonds : $1 - 10 \quad 3 - 11 \quad 4 - 7 \quad 5 - 8 \quad 6 - 9 \quad 13 - 15 \quad 15 - 39 \quad 15 - 40 \quad 15 - 41 \quad 16 - 25 \quad 17 - 26 \quad 19 - 22 \quad 20 - 23 \quad 21 - 24 \quad 27 - 28 \quad 27$ 29-33 31-32 33-36 33-37 33-38 normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21 \quad 29-30 \quad 29-31$ Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS fragments assigned product role: containing 1 fragments assigned reactant/reagent role: containing 16

containing 29

15:33 13:29 14:30 2:18

node mappings: